

2,2,2-Trifluoroethanol  
75-89-8 | DTXSID0021751

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

## Model Results

**Predicted value:** 12.7 L/kg

**Global applicability domain:** Inside

**Local applicability domain index:** 5.79e-01

**Confidence level:** 7.89e-01

## Nearest Neighbors from the Training Set

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Methyl isothiocyanate

**Measured:** 9.33

**Predicted:** 7.63

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Epichlorohydrin

**Measured:** 10.0

**Predicted:** 9.87

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Thioacetamide

**Measured:** 6.03

**Predicted:** 6.43

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1,2-Dichloroethane

**Measured:** 33.1

**Predicted:** 32.5

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Pyridine

**Measured:** 39.8

**Predicted:** 20.1